Condensation of N interacting bosons: Hybrid approach to condensate fluctuations

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We present a new method of calculating the distribution function and fluctuations for a Bose-Einstein condensate (BEC) of N interacting atoms. The present formulation combines our previous master equation and canonical ensemble quasiparticle techniques. It is applicable both for ideal and interacting Bogoliubov BEC and yields remarkable accuracy at all temperatures. For the interacting gas of 200 bosons in a box we plot the temperature dependence of the first four central moments of the condensate particle number and compare the results with the ideal gas. For the interacting mesoscopic BEC, as with the ideal gas, we find a smooth transition for the condensate particle number as we pass through the critical temperature.

Bose-Einstein condensation (BEC) near the critical temperature T_c is a fascinating subject. Indeed the time line from the early studies of Uhlenbeck [1] concerning the unphysical cusp at T_c in Einstein's analysis, to the "Grand canonical catastrophe" [2], arising from ill fated attempts to describe fluctuations [3], covers most of the twentieth century. Naturally, a major stimulus for the present work is the pioneering BEC experiments in liquid He-II [4] and in laser cooled gases [5]. The attendant theoretical advances in the study of BEC in ideal and interacting gases likewise constitute a rich field [6, 7].

Furthermore, subtle issues such as the statistics of condensate atoms in a mesoscopic system of $N \sim 10^2 - 10^3$ particles are now of interest. Condensate fluctuations can be measured by means of a scattering of series of short laser pulses [8], see also [9]. We note that the BEC is often referred to as an atom laser; indeed the problem of BEC statistics near T_c is analogous to studying the photon statistics of the laser in the passage from below to above threshold [10, 11].

In the present Letter, we give, for the first time, a simple, surprisingly accurate account of fluctuations in an interacting Bogoliubov gas valid for all temperatures. We omit, however, effects of interaction between Bogoliubov quasiparticles since we treat a weakly interacting gas. The analysis is based on a master equation approach deriving from a union of the ideal gas (in the spirit of the quantum theory of the laser) BEC treatment of the first two papers in this series on the condensation of N bosons [10] and the results for the interacting gas BEC obtained based on the canonical ensemble quasiparticle formalism [12].

We emphasize that although useful papers have been published dealing with various limiting cases, so far there has been no treatment of this problem valid at all temperatures [3]. Ref. [12] presented analytical formulas for all moments of the condensate particle number fluctuations in the weakly interacting Bose gas. However, [12] and other approaches (e.g. Ref. [13]) are only valid provided the average number of condensate particles is much larger than its variance. However, near and above T_c this is not true, and this causes the failure of such treatments.

For an ideal Bose gas the master equation approach

of [10] naturally includes the N particle constraint and provides an analytical solution for the partition function and fluctuations accurate at all temperatures, as shown in Fig. 1. For an interacting gas, the problem of fluctuations is rather delicate. In a recent paper [15] we gave a preliminary master equation analysis for N interacting atoms which accurately described the average number of particles in the condensate. However the fluctuations were handled less well. The present analysis gives all central moments with remarkable accuracy when compared to [12] below T_c. Above T_c the present results go smoothly into the ideal gas limit as they must.
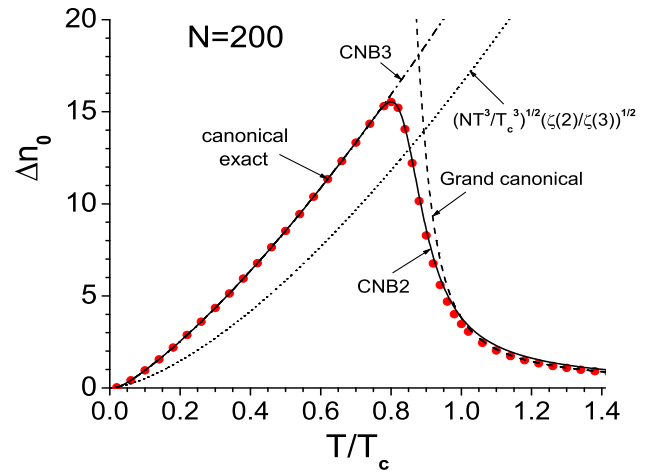

FIG. 1: The variance for the condensate particle number as a function of temperature for an ideal gas of $N = 200$ particles in an isotropic harmonic trap obtained by the master equation approach of [10] (solid line), "exact" numerical simulations in the canonical ensemble (dots) and the grand canonical answer (dashed line). Result of Refs. [2, 12] is plotted as dash-dot line. Small dots show the thermodynamic limit formula of Politzer [14].

The central tool used in the ideal gas analysis of [10] and the interacting gas study of [15] was the laser-like

master equation for the probability p_{n_0} of finding n_0 atoms in the condensate, given that there are N total particles

$$\frac{1}{\kappa}\dot{p}_{n_0} = -K_{n_0}(n_0 + 1)p_{n_0} + K_{n_0-1}n_0 p_{n_0-1} -$$

$$H_{n_0}n_0 p_{n_0} + H_{n_0+1}(n_0 + 1)p_{n_0+1}, \qquad (1)$$

where κ is an uninteresting rate constant, H_{n_0} and K_{n_0} are heating and cooling coefficients. In equilibrium the rates of any two opposite processes are equal to each other, e.g., $K_{n_0}(n_0 + 1)p_{n_0} = H_{n_0+1}(n_0 + 1)p_{n_0+1}$. The detailed balance condition yields

$$\frac{p_{n_0+1}}{p_{n_0}} = \frac{K_{n_0}}{H_{n_0+1}}. \qquad (2)$$

Since the occupation number of the ground state cannot be larger than N there is a canonical ensemble constraint $p_{N+1} = 0$ and, hence, $K_N = 0$. In contrast to p_{n_0}, the ratio p_{n_0+1}/p_{n_0} as a function of n_0 shows simple monotonic behavior. We approximate K_{n_0} and H_{n_0} by a few terms of the Taylor expansion near the point $n_0 = N$

$$K_{n_0} = (N - n_0)(1 + \eta) + \alpha(N - n_0)^2, \qquad (3)$$

$$H_{n_0} = \mathcal{H} + (N - n_0)\eta + \alpha(N - n_0)^2. \qquad (4)$$

Parameters $\mathcal{H}$, η and α are independent of n_0; they are functions of the occupation of the excited levels. We derive them below by matching the first three central moments in the low temperature limit with the result of [12]. We note that the detailed balance equation (2) is the Padé approximation [16] of the function p_{n_0+1}/p_{n_0}. Padé summation has proven to be useful in many applications, including condensed-matter problems and quantum field theory.

Eqs. (2)-(4) yield an analytical expression for the condensate distribution function

$$p_{n_0} = \frac{1}{\mathcal{Z}_N}\frac{(N - n_0 - 1 + x_1)!(N - n_0 - 1 + x_2)!}{(N - n_0)!(N - n_0 + (1 + \eta)/\alpha)!}, \quad (5)$$

where $x_{1,2} = (\eta \pm \sqrt{\eta^2 - 4\alpha\mathcal{H}})/2\alpha$ and $\mathcal{Z}_N$ is the normalization constant determined by $\sum_{n_0=0}^{N} p_{n_0} = 1$. In the particular case $\eta = \alpha = 0$ Eq. (5) reduces to

$$p_{n_0} = \frac{1}{Z_N}\frac{\mathcal{H}^{N-n_0}}{(N - n_0)!}, \qquad (6)$$

where $Z_N = e^{\mathcal{H}}\Gamma(N + 1, \mathcal{H})/N!$ is the partition function and Γ is an incomplete gamma-function. For an ideal gas Eq. (6) describes accurately the condensate statistics at low temperature [10]. The statistics is not Poissonian

$p_n = \bar{n}^n e^{-\bar{n}}/n!$, as would be expected for a coherent state.

Using the distribution function (5) we find that, in the validity range of [12] (at low T), the first three central moments $\mu_m \equiv\, <(n_0 - \bar{n}_0)^m>$ are

$$\bar{n}_0 = N - \mathcal{H}, \qquad \mu_2 = (1 + \eta)\mathcal{H} + \alpha\mathcal{H}^2, \qquad (7)$$

$$\mu_3 = -\mathcal{H}(1 + \eta + \alpha\mathcal{H})(1 + 2\eta + 4\alpha\mathcal{H}). \qquad (8)$$

Eqs. (7), (8) thus yield

$$\mathcal{H} = N - \bar{n}_0, \qquad \eta = \frac{1}{2}\left(\frac{\mu_3}{\mu_2} - 3 + \frac{4\mu_2}{\mathcal{H}}\right), \qquad (9)$$

$$\alpha = \frac{1}{\mathcal{H}}\left(\frac{1}{2} - \frac{\mu_2}{\mathcal{H}} - \frac{\mu_3}{2\mu_2}\right). \qquad (10)$$

On the other hand, the result of [12] for an interacting Bogoliubov gas is (see also [13] for $\bar{n}_0$ and μ_2)

$$\bar{n}_0 = N - \sum_{k\neq 0}\left[\left(u_k^2 + v_k^2\right)f_k + v_k^2\right], \qquad (11)$$

$$\mu_2 = \sum_{k\neq 0}\left[(1 + 8u_k^2 v_k^2)(f_k^2 + f_k) + 2u_k^2 v_k^2\right], \qquad (12)$$

$$\mu_3 = -\sum_{k\neq 0}\left(u_k^2 + v_k^2\right)\left[(1 + 16u_k^2 v_k^2)(2f_k^3 + 3f_k^2 + f_k) + \right.$$

$$\left. 4u_k^2 v_k^2(1 + 2f_k)\right], \qquad (13)$$

where $f_k = 1/[\exp(E_k/k_B T) - 1]$ is the number of elementary excitations with energy E_k present in the system at thermal equilibrium, u_k and v_k are Bogoliubov amplitudes. Substitute for $\bar{n}_0$, μ_2 and μ_3 in Eqs. (9), (10) their expressions of Ref. [12] (11)-(13) yields the unknown parameters $\mathcal{H}$, η and α. The beauty of our "matched asymptote" derivation is that the formulas for $\mathcal{H}$, η and α are applicable at all temperatures, i.e. not only in the validity range of [12]. The distribution function (5) together with Eqs. (9), (10) provides complete knowledge of the condensate statistics at all T. Taking $v_k = 0$ and $u_k = 1$ in (11)-(13) we obtain the ideal gas limit.

Next we test our method for an ideal gas (in a harmonic trap). In this case an "exact" numerical simulation in the canonical ensemble [7] is available for comparison. Results of such simulation are shown by dots in Figs. 2 and 3. In Fig. 2 we plot the distribution function for the number of atoms in condensate at different temperatures and $N = 200$. At $T \ll T_c$ the distribution shows a sharp peak near $\bar{n}_0$ and becomes broader at

higher T. The present Eq. (5) (solid line) yields excellent agreement with the "exact" dots at all temperatures. Fig. 3 shows the average condensate particle number $\bar{n}_0$, its variance, third and fourth central moments μ_m and fourth cumulant κ_4 [17] as a function of T for $N = 200$ particles in a harmonic trap. Solid lines are the result of the present approach (we call it CNB5 [18]) which is in remarkable agreement with the "exact" dots at all temperatures both for μ_m and κ_4. Central moments and cumulants higher than fourth order are not shown here, but they are also remarkably accurate at all temperatures. Results of [12] are given by dashed lines which are accurate only at sufficiently low T. Deviation of higher order cumulants $(m = 3, 4, \ldots)$ from zero indicates that the fluctuations are not Gaussian.
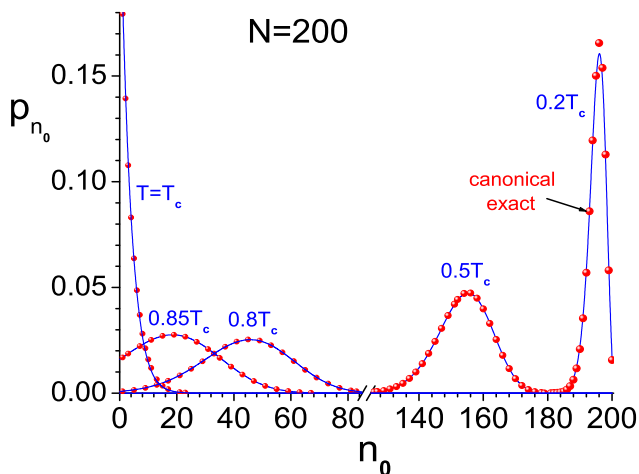

FIG. 2: Distribution function for the condensate particle number n_0 at different temperature obtained by the present approach (solid lines) and "exact" numerical simulations in the canonical ensemble (dots). The results are obtained for an ideal gas of $N = 200$ particles in an isotropic harmonic trap.

Clearly our method passes the ideal gas test with flying colors. Please note the excellent agreement with the exact analysis for the third central moment and fourth cumulant κ_4 given in Fig. 3.

Next we apply the present technique to N interacting Bogoliubov particles confined in a box of volume V. The interactions are characterized by the gas parameter $an^{1/3}$, where a is the s-wave scattering length and $n = N/V$ is the particle density. The energy of Bogoliubov quasiparticles E_k depends on $\bar{n}_0$, hence, the equation $\bar{n}_0 = \sum_{n_0=0}^{N} n_0 p_{n_0}$ for $\bar{n}_0$ must be solved self-consistently. In Fig. 4 we plot $\bar{n}_0$, the variance Δn_0, third and fourth central moments as a function of T for an ideal and interacting $(an^{1/3} = 0.1)$ gas in the box. Solid lines show the result of the present approach, while [12] is represented by dashed lines. The present results agree well for all μ_m with [12] in the range of its validity. Near and above T_c [12] becomes inaccurate. However, the results of the present method are expected to be accurate at all T. Indeed, in the limit $T \gg T_c$ the present results (unlike [12]) merge with those for the ideal gas. This is physically appealing since at high T the kinetic energy becomes much larger than the interaction energy and the gas behaves ideally. Similar to the ideal gas, the interacting mesoscopic BEC $\bar{n}_0(T)$ exhibits a smooth transition when passing through T_c.

One can see from Fig. 4 that the repulsive interaction stimulates BEC, and yields an increase in $\bar{n}_0$ at intermediate temperatures, as compared to the ideal gas. This effect is known as "attraction in momentum space" and occurs for energetic reasons [19]. Bosons in different states interact more strongly than when they are in the same state, and this favors multiple occupation of a single one-particle state.

In conclusion, in this paper we presented a simple method which, for the first time, yields an accurate description of the distribution function and fluctuations for mesoscopic interacting Bogoliubov BEC in the canonical ensemble at all temperatures. Our approach combines the analytical results of [12] with the laser-like master equation of [15].

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[18] The present paper is the fifth in the series of our Condensation of N Bosons papers.
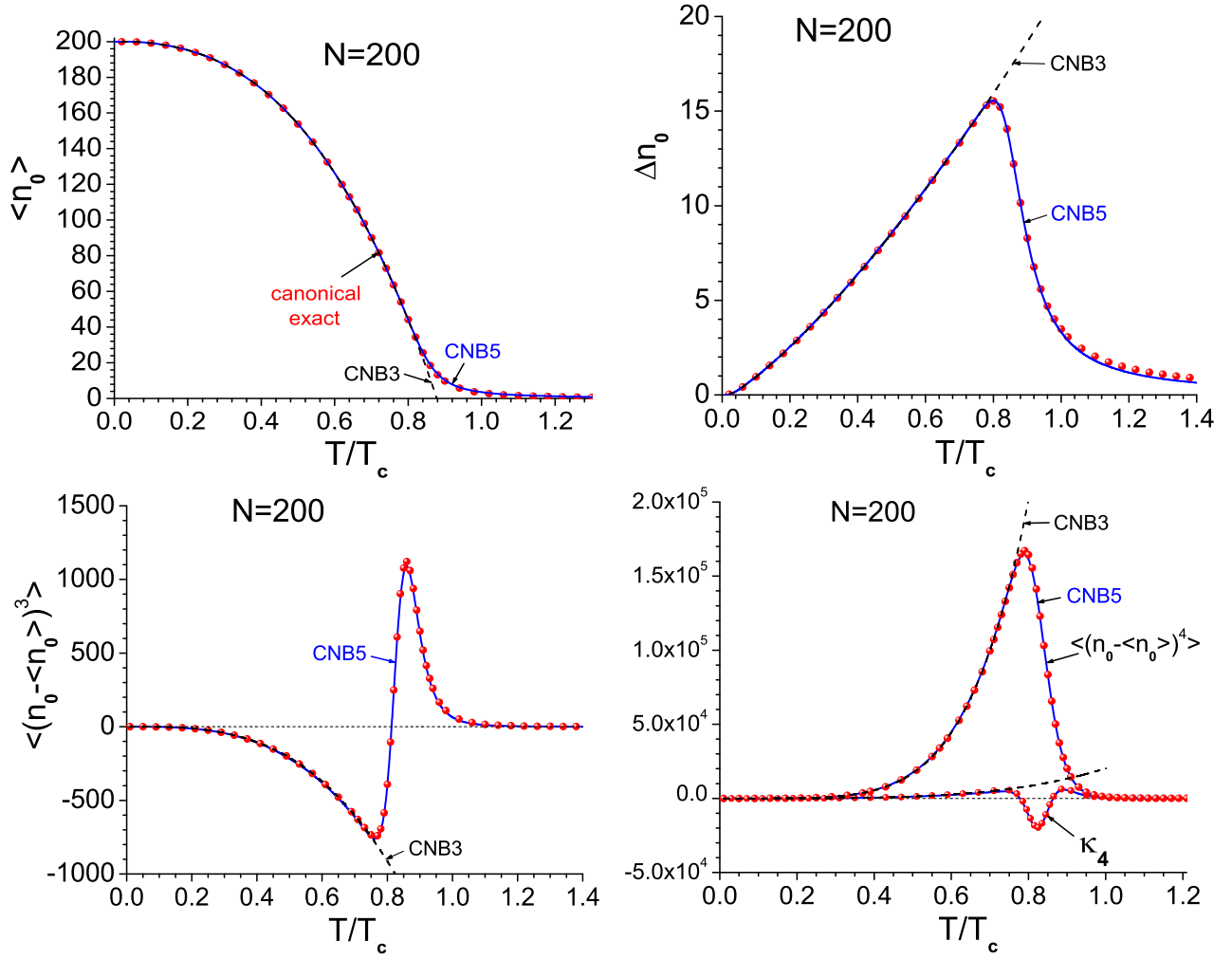
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FIG. 3: Average condensate particle number $< n_0 >$, its variance $\Delta n_0 = \sqrt{< (n_0 - \bar{n}_0)^2 >}$, third and fourth central moments $< (n_0 - \bar{n}_0)^m > (m = 3, 4)$ and fourth cumulant κ_4 as a function of temperature for an ideal gas of $N = 200$ particles in a harmonic trap. Solid lines (CNB5) show the result of the present approach. [12] yields dashed lines (CNB3). Dots are "exact" numerical simulation in the canonical ensemble. The temperature is normalized by the thermodynamic critical temperature for the trap $T_c = \hbar \omega N^{1/3}/k_B \zeta(3)^{1/3}$, where ω is the trap frequency.
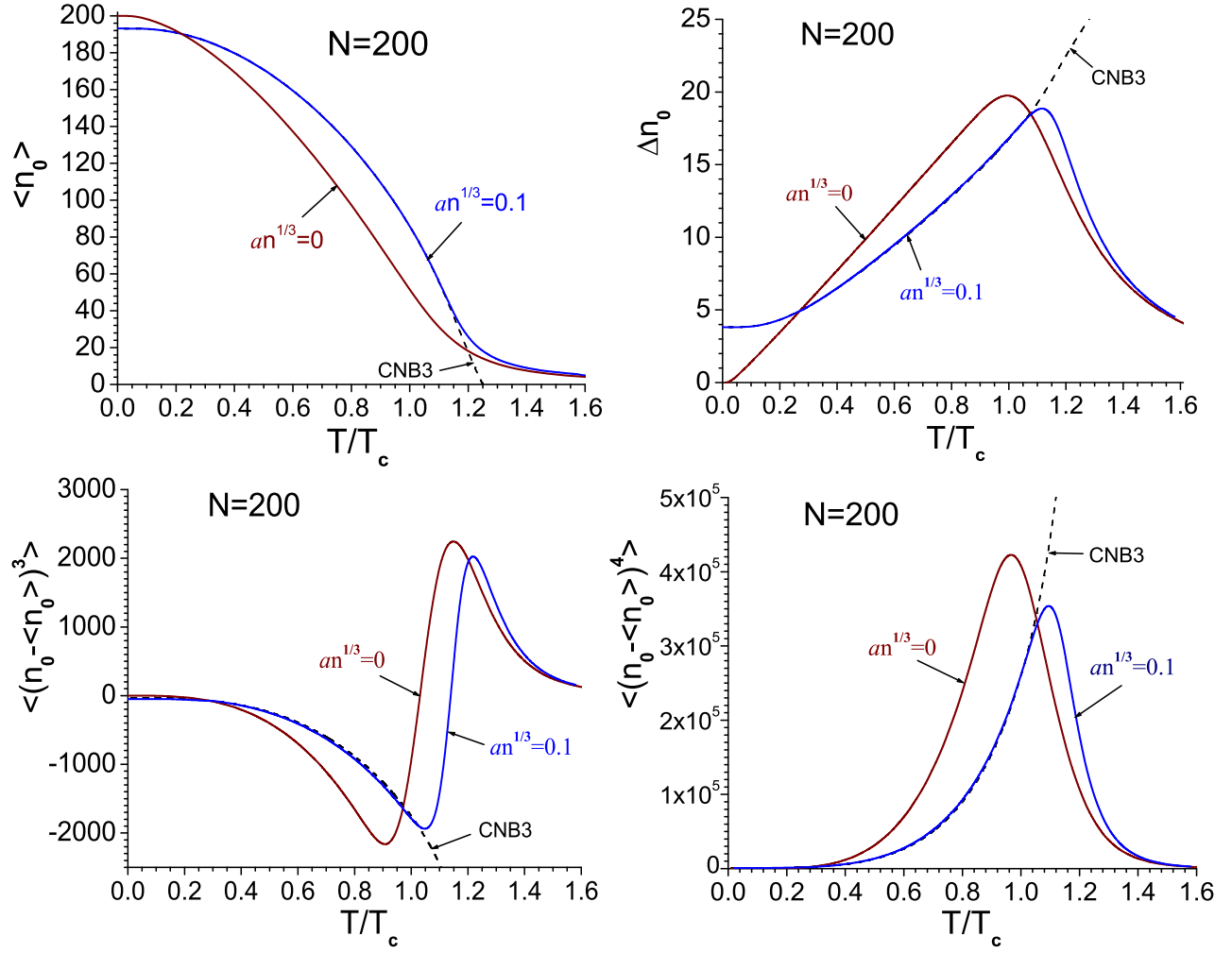
FIG. 4: Average condensate particle number, its variance, third and fourth central moments as a function of temperature for an ideal ($an^{1/3} = 0$) and interacting ($an^{1/3} = 0.1$) Bose gas of $N = 200$ particles in a box. Solid lines are the result of the present approach. [12] yields dashed lines (CNB3). The temperature is normalized by the thermodynamic critical temperature for the box $T_c = 2\pi\hbar^2 n^{2/3}/k_B M\zeta(3/2)^{2/3}$, where M is the particle mass.